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ATOMIC ARRANGEMENTS AND ELECTRONIC PROPERTIES OF SEMICONDUCTOR --ETC(U)
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November 1, 1980 - October 31, 1981

**"Atomic Arrangements and Electronic Properties
of Semiconductor Surfaces and Interfaces"**

by

D. J. Chadi and Richard. M. Martin

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SUMMARY OF RECENT WORK

The areas of research during the past 12 months have included: (i) step-formation energies and domain orientation at Si(111) surfaces; (ii) the electronic structure of the Al-GaAs(110) surface chemisorption system; (iii) density-functional calculations of bulk properties of GaAs and of (100)GaAs-Ge interfaces; (iv) demonstration of the importance of correlation effects on the atomic and electronic structure of Si(111) surfaces; and (v) derivation of an exact scaling law for the resistance of a thin wire for the one-dimensional Anderson model containing both diagonal and off-diagonal disorder.

Personnel Involved and Their Home Institutions

D. J. Chadi	Principal Investigator, Xerox
R. M. Martin	Co-Principal Investigator, Xerox On sabbatical leave at the University of Paris (Sept. 1980 - Sept. 1981)

Visiting Scientists:

R. Del Sole	Jan. 1981 - Jan. 1982, University of Rome
J. D. Joannopoulos	Jan. 1981, M.I.T.
R. Haydock	June 22 - Aug. 21, 1981, Cavendish Laboratory, England
J. Ihm	June 22 - Aug. 21, 1981, M.I.T.
C. Tanner	July 1 - Sept. 15, 1981, University of California, Berkeley
Y. Petroff	Sept. 1 - 15, 1981, University of Paris, Orsay

Collaborators Abroad:

K. Kunc	University of Paris VI, Paris
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Recent Publications

1. "New c-2x8 Unit Cell for the Ge(111) Surface," D. J. Chadi and C. Chiang, Phys. Rev. B 23, 1843 (1981).
2. "Theoretical Studies of Si(111) Surfaces," D. J. Chadi, J. Vac. Sci. Technol. 18, 856 (1981).
3. "Electronic Structure of the Al-GaAs (110) Surface Chemisorption System," J. R. Chelikowsky, D. J. Chadi, and M. L. Cohen, Phys. Rev. B 23, 4013 (1981).
4. "Reconstruction at Semiconductor Surfaces," D. J. Chadi, J. Phys. Soc. Japan 49, Suppl. A, 1035 (1980).
5. "Relaxation of Polar Ge-GaAs(100) Interfaces: Self-Consistent Calculations of the Total Energy," K. Kunc and R. M. Martin, J. Phys. Soc. Japan 49, Suppl. A, 1117 (1980).
6. "Direct Method of Calculation of Dynamic Effective Charges: Application to GaAs," R. M. Martin and K. Kunc, Phys. Rev. B 24, 2081 (1981).
7. "Density Functional Calculation of Structure and Lattice Dynamics of GaAs," K. Kunc and R. M. Martin, Phys. Rev. Rapid Commun. B 24, 2311 (1981).

Papers Submitted for Publication

1. "Step-Formation Energies and Domain Orientation at Si(111) Surfaces," D. J. Chadi, J. R. Chelikowsky, Phys. Rev. B 24, Rapid Communications, Oct. 1981.
2. "Correlation Effects on the Electronic Structure of 1x1 and 2x1 Reconstructed Si (111) Surfaces," R. Del Sole and D. J. Chadi (to be published).
3. "Scaling Studies of the Resistivity of the One-Dimensional Anderson Model with General Disorder," D. A. Stone, J. D. Joannopoulos, and D. J. Chadi, Phys. Rev. B 24 (to be published).

4. "Comments on Computational Methods for Structural Energies of Semiconductors," R. M. Martin and K. Kunc, Proceedings of the CECAM Workshop on Ab Initio Calculation of Phonon Dispersion, Antwerp, June 1981.
5. "Lattice Dynamics of GaAs.," K. Kunc and R. M. Martin, Proceedings of the CECAM Workshop on Ab Initio Calculation of Phonon Dispersion, Antwerp, June 1981.
6. "Recent Advances in the Theory of Phonons in Semiconductors," R. M. Martin, Proceedings of the International Conference on Phonon Physics, Bloomington, IN, Sept. 1981.
7. "Ab Initio Force Constants in Ge," K. Kunc and R. M. Martin, Proceedings of the International Conference on Phonon Physics, Bloomington, IN, Sept. 1981.
8. "Ab Initio Force Constants of GaAs: A New Approach to Calculation of Phonons and Dielectric Properties" K. Kunc and R. M. Martin, submitted to Phys. Rev. Letters.

Research Report

The primary area of our research continues to be on semiconductor surfaces and interfaces. A variety of systems were studied using both tight-binding and self-consistent pseudopotential methods. In the following, we present a brief exposition of the progress we have made during the course of the past year (Nov. 1, 1980 - Oct. 31, 1981).

1. *Stepped Si(111) Surfaces.* Steps are a low energy defect structure at the surface. Two distinct types of steps can occur on the Si(111) surface. The primary difference between the two is in the number of broken bonds at step atoms. One configuration has two broken bonds per step atom, the other only one broken bond. Experimentally only two broken-bond geometries are observed on cleaved Si(111) surfaces. The greater stability of the two broken bond configuration has been a puzzle since its discovery in about 1968. A simple three-part explanations for this puzzle was derived. These consist of: (i) Step-creation reduces the number of surface dangling bonds because the steps are not sharp but have a finite dimension. The reduction in the surface dangling-bond density is different for the two-step configurations. The two-broken-bond geometry reduces the surface dangling-bond density twice as fast as the one-broken bond geometry. This important difference between the two types of step configurations had been apparently ignored in the past. (ii) The energy required to create two dangling bonds on an atom is always less than twice the energy to create a single broken bond. The reason for this is that the two broken dangling bonds rehybridize to lower their energy. In Si the rehybridization from sp^3 to sp at step atom results in an energy release of about 1.5eV. (iii) Reconstruction and relaxation effects result in a further reduction of the total energy. Combining steps (i) to (iii), the difference in the cleavage energies of the surface with the two different step-configurations was calculated. Cleavage and vacancy formation energies were also determined. It was shown that steps form a low-energy defect structure at the surface. The problem of domain orientation at steps and of atomic reconstruction were studied in detail. Two inequivalent domain orientations with differing electronic structures were shown to be energetically favorable at the surface. Low-energy-electron-diffraction studies support this conclusion. This work was done by D. J. Chadi in collaboration with J. R. Chelikowsky.
2. *Al-GaAs(110) Chemisorption System.* In this work, we have examined a new model for the $\frac{1}{2}$ -monolayer chemisorption of Al on the GaAs surface. The primary bonding of Al was taken to be to the cation site instead of to

the anion site, as suggested by recent quantum-chemical calculations on clusters. The self-consistent pseudopotential method was used to analyze the surface electronic bands and charge densities for this geometry. The results were found to be compatible with the available experimental data from photoemission, surface photovoltage spectroscopy and core shifts on unannealed surfaces. Low-energy-electron-diffraction, as well as energy-minimization studies suggest that upon annealing of the surface an exchange reaction between Al and substrate Ga atoms takes place. The surface dipole of Al chemisorbed on *intrinsic* GaAs was found to be positive. The negative dipole observed experimentally is suggested to be a consequence of employing an n-type sample and is not the intrinsic dipole. This work was done by D. J. Chadi in collaboration with J. R. Chelikowsky and M. L. Cohen.

3. *Ab Initio Calculations of Structural Properties: Bulk Crystals.* Self-consistent density functional calculations have been developed to calculate directly total energies as a function of positions of the atoms. The first application of these methods involves bulk crystals and provides a very severe and convincing test that structural energies can be calculated accurately with no adjustable parameters. For example, in GaAs the lattice constant, phonon frequencies, Gruneisen parameters, are all calculated with good agreement with experiment. Our primary efforts this year have been to examine *difficult* bulk properties that are directly related to the important properties of surfaces and interfaces discussed below. These are problems of large displacements and Coulomb fields. For GaAs we have found that large displacements corresponding to the TA(X) can become unstable in some situations, which shows that such extreme anharmonic efforts are potentially very important at surfaces or interfaces. The problem of Coulomb fields requires very careful analysis which we have now done to show that effective changes can be calculated directly. This is an important result in itself and, in addition, is an exacting test of our techniques for handling the problems that appear in surfaces or interfaces. Two papers have been published and four are in press. This work was done by K. Kunc and R. M. Martin.
4. *Ab Initio Calculations of Interface Properties: Ge:GaAs.* The basic problems in understanding surfaces and interfaces is to predict the atomic structure. The covalently bonded semiconductors are particularly interesting because the equilibrium structure apparently always involves large atomic displacements and new bonding situations totally different from any known bulk cases. This is just the type of problem where accurate *ab initio* calculations can have the most impact and indeed can expand our knowledge. We have chosen to work on the Ge-GaAs system

because our previous work indicated that the low energy structures could be clearly classified and investigated. In particular, it was shown that interface layers should have mixed Ge-Ga and/or Ge-As stoichiometry. The foremost question is the chemical stoichiometry and topology of the interface, with the exact positions of the atoms as a secondary issue. We have carried out density functional calculations within the approximation of averaging atoms in mixed layers. This is an important first step in proceeding with the calculations and gives much information on properties, such as work functions, etc. The next steps in our future work are to consider the interface layers more accurately and predict the most favorable stoichiometries and reconstructions. This work was done by R. M. Martin and K. Kunc.

5. *Correlation Effects on Surfaces.* Electron-electron correlations are not always explicitly included in studying the electronic properties of semiconductors, because with some exceptions, they are not generally found to lead to big effects. We have recently shown that electron-electron correlations do have a large effect on the electronic structure of the Si(111) surface. In particular, such correlations lead to a new electronic phase for the 2×1 surface which differs very significantly from the previously accepted picture of the surface electronic structure. The electronic properties of the new phase are in good agreement with experiments and leads to a resolution of several outstanding problems, e.g., (i) photoemission measurements of band positions are explained and reconciled with optical data on band gaps for the first time; (ii) Fermi-level pinning position is correctly given; (iii) core-shifts are in much better agreement with experiment; and (iv) the discrepancy between LEED structure versus theoretical structures is removed. More work in this area is in progress. This work is done by D. J. Chadi in collaboration with R. Del Sole.
6. *Random Systems.* The problem of electron localization in one-dimension resulting from disorder was studied by D. J. Chadi in collaboration with J. D. Joannopoulos and D. Stone. The exact dependence of the "scale-resistance" to fluctuations in both atomic self-energies and matrix-elements were derived. This is the first time that both effects have been considered simultaneously. The scale resistance corresponds to the resistance of a length of wire over which the electron scattering from site to site is elastic. The measured resistance is an ensemble average of the scale resistance over many inelastic scattering lengths. By going to very low temperatures where the inelastic scattering length can be made large, drastic effects in the resistivity of thin wires are expected to occur and have in fact been observed experimentally. Our calculations show that the scale resistance grows exponentially with length. The probability distribution of the

resistance as a function of the statistical fluctuations was derived. The results were also tested via extensive computer simulations of a random one-dimensional network. The analytical method of solution relies on powerful new mathematical methods which should also prove useful in surface and interface problems.